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NLR-TP-98234

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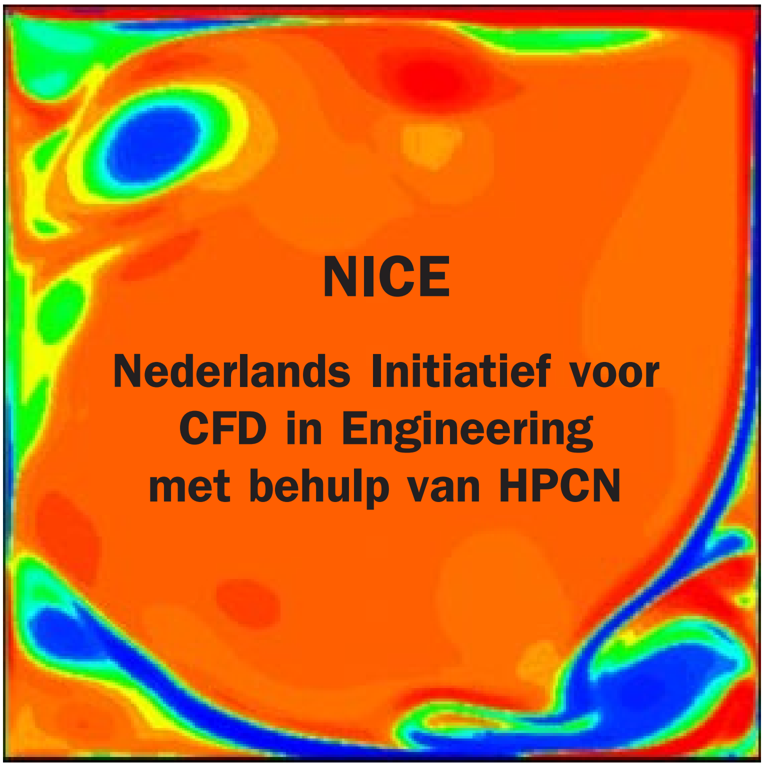

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The work described in this report is partially supported by the Dutch Foundation HPCN in the project NICE under contract number 96009.

This report is based on a presentation to be held on the ECCOMAS '98 conference, Athens, Greece, 7-11 September 1998.

Division: Informatics
Issued: May 1998
Classification of title: unclassified

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Summary

In this study a software tool for generic design optimization involving CFD analysis is developed. A multi-purpose optimization routine of the NAG Fortran Library, employing a sequential quadratic programming method, is used. The objective function, which depends on the CFD results, and its sensitivities, which are required by the optimization algorithm, are computationally expensive to evaluate. To achieve optimal performance and maximum flexibility, the optimization tool uses a CFD solver that is specifically suited for the considered CFD problem and optimized for execution on the applied hardware platform -an NEC SX-4/16 super computer. Extra speed-up of the optimization process is achieved by parallelization of the calculations of the objective function and sensitivities.

1 Introduction

CFD analysis can aid in the process of product design by predicting whether a product will meet certain requirements. However, it is becoming increasingly desirable that not only the requirements are met, but also that certain properties of the product are optimized during the design process. For this purpose use can be made of numerical optimization procedures.

Optimization algorithms minimize non-linear objective functions iteratively. Usually these algorithms require frequent evaluation of the objective function. In the case of design optimization involving CFD analysis the objective function is based on the CFD results, which are in general computationally expensive to obtain. Many optimization algorithms make use of the sensitivity of the objective function to the design parameters 3. The sensitivities of the CFD results, and consequently of the objective function, to the design parameters are usually not a priori known and can not be derived analytically. Therefore finite difference techniques are used to approximate these sensitivities. The computational cost of the calculation of the sensitivities is proportional to the number of design parameters.

The aim of this study is to develop a software tool for generic design optimization involving CFD analysis. This tool must be applicable to a wide class of CFD problems and must have optimal performance. For these purposes the optimization tool uses the CFD solver that is most suitable to the considered CFD problem. The CFD simulations are run on the NEC SX-4 16 processor parallel vector computer of NLR with a theoretical peak performance of 2 Gflop/s per processor. Readily available CFD solvers optimized for this platform can be selected by the user. To achieve a wide applicability and robust behaviour of the optimization tool, a multi-purpose optimization routine of the NAG Fortran Library is used. This routine is based on a sequential quadratic programming (SQP) method incorporating an augmented Lagrangian merit function of the objective function and a quasi-Newton approximation to the Hessian of the Lagrangian merit function 1, 2. To speed-up the calculation of the objective function and its sensitivities in each optimization iteration, the required CFD simulations are run in parallel.

In this paper a brief description of the optimization tool is given. To illustrate the genericness and performance of the tool, two totally different design optimization studies will be presented. One study concerns the optimal design of an industrial air heating system. The other concerns the geometric optimization of a 2-D airfoil. The resulting optimization iterations, optimal designs and computational performances will be presented and discussed.

2 The Optimization Tool

The optimization tool is used to determine the values of certain design parameters of a product, such that certain properties of the product are optimized according to the requirements of the user. This is achieved by minimization of a user defined objective function which reflects the desired properties of the product. The objective function is expressed as a function of CFD results.

The optimization tool consists of a number of program units that run on different platforms (fig. 1). The CFD simulations for the computation of the objective function and the sensitivities are run on the SX-4 super computer. Because of the very limited computational costs of the optimization program and the program manager, these program units are run on a workstation. The modular program structure permits easy extendability of the program units and re-use and exchange of dedicated software. The program units are executed by the program manager via readily available

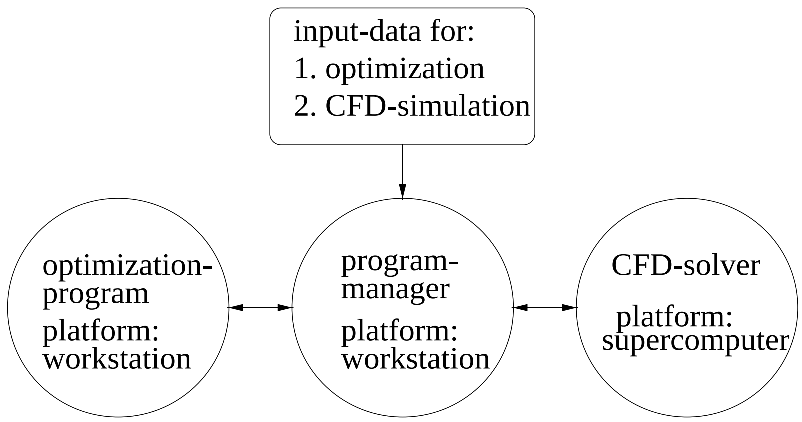


Fig. 1 Program structure of the optimization tool

tool wrappers 4, which account for the correct input and output data transmission and batch job queueing.

The input data for the optimization tool is specified by the user and consists of two data sets. In one data set the specifications for the optimization are given. The other data set consists of the parameterized input data for the CFD solver, in which the flow problem is defined and the design parameters are incorporated. The latter data set is specific for the CFD solver that is used.

The objective function F is constructed from the CFD results r, such as for example velocity and pressure, which depend on the design parameters p:

$$F(p) = \frac{1}{2} \sum_{k=1}^{m_2} \sum_{j=1}^{m_1} [w_k(d_k - r_{j,k}(p))]^2 \tag{1}$$

m_2 is the number of result types and m_1 is the number of results per type that are used in the objective function. w and d are the weightfactors and the desired values, respectively, for each result type. The set of n design parameters p is subject to the constraints:

$$b_i^l \leq p_i \leq b_i^u \quad ; \quad i = 1, \ldots, n \tag{2}$$

3 Design Optimization of an Air Heater

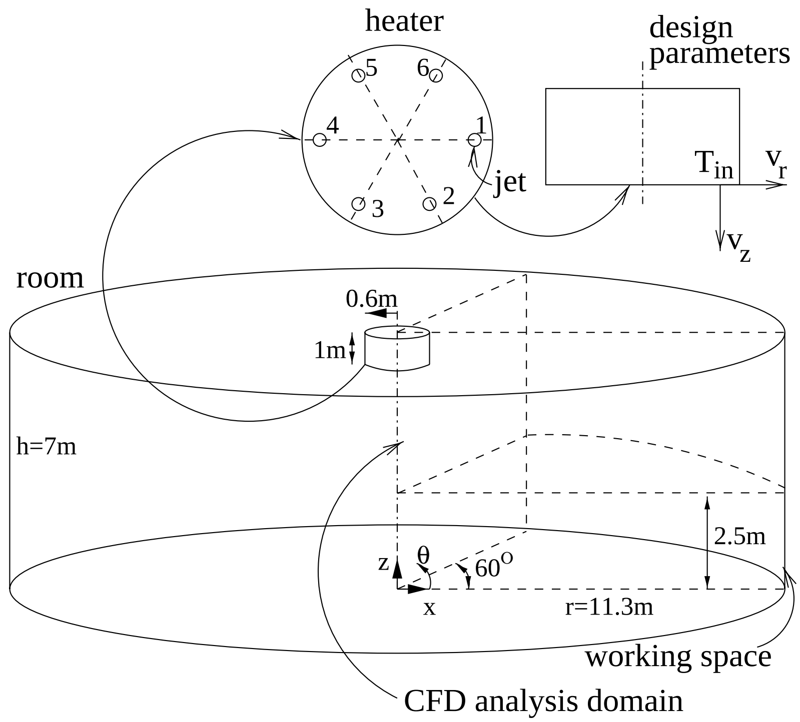


Fig. 2 The industrial heater system

As an illustration of the use of the optimization tool, an optimization study of the design of an industrial air heating system is presented. This system consists of a hot air blower with 6 jets, attached to the ceiling of a 7 m high room and intended to heat a working space of about 400 m^2 and 2.5 m high (fig. 2). The objective in this optimization is to design the heating system such that the hot jets heat up the working space to a desired temperature, without inducing high air flow velocities in the working space. The design parameters are the radial velocity (v_r), vertical velocity (v_z) and the temperature (T_{in}) of the jets, which are prescribed as boundary conditions. Initial estimates and lower and upper bounds are 10 m/s, 0 m/s and 30 m/s, respectively, for v_r, -10 m/s, -30 m/s and 0 m/s, respectively, for v_z, and 300 K, 290 K and 350 K, respectively, for T_{in}. Slip and adiabatic boundary conditions are prescribed at the boundaries θ=0, θ=π/3 and r=11.3 m. Slip and T=288 K is prescribed at the boundaries z=0 m and z=7 m, and at the latter also a heat conduction coefficient of 4.17 J/(K m^2) is prescribed to allow energy losses through the ceiling. The governing equations are the continuity equation, momentum equation and the energy equation for incompressible flow 6, 5. The $k-\epsilon$ turbulence model is used. Buoyancy effects occur due to the temperature dependent air density: ρ=1.209 [1-0.0035(T-291)]; ρ in kg/m^3 and T in K. Gravitational acceleration is g=9.81 m/s^2. A cylindrical Cartesian 25$\times$6$\times$25-grid of the CFD analysis domain of 11.3 m $\times$ π/3 $\times$ 7 m has been used. The flow simulation is performed with

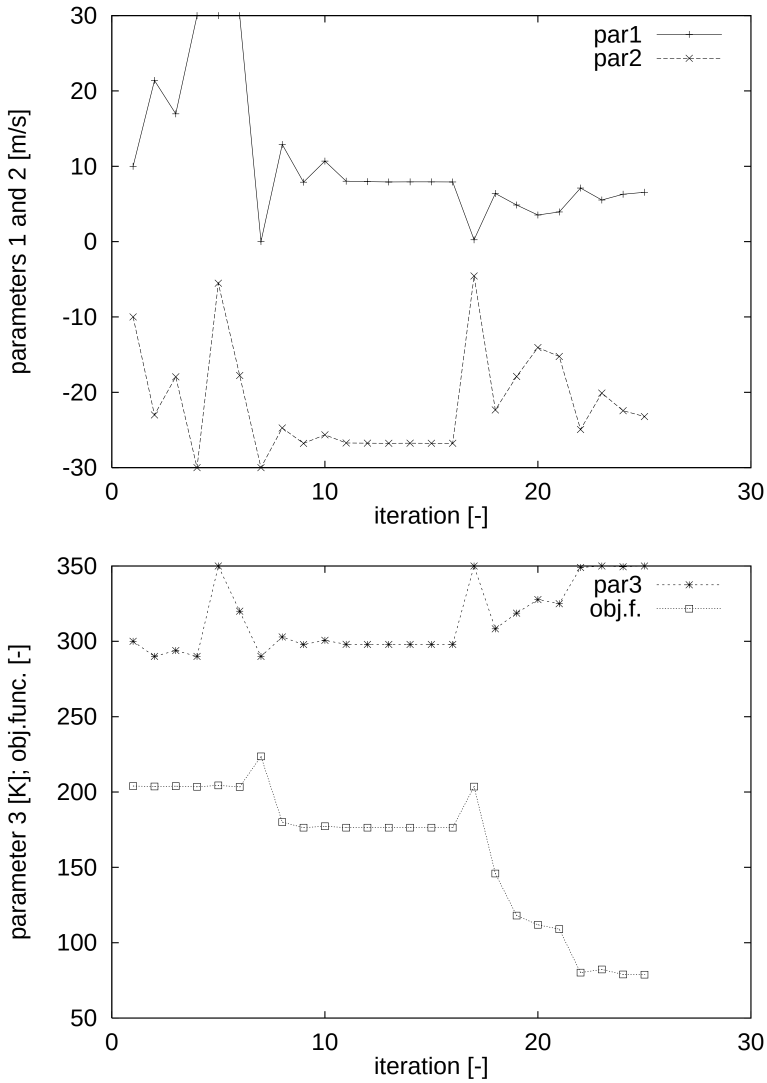


Fig. 3 Design parameters v_r and v_z (par1 and par2 in upper panel) and T_{in} and objective function (par3 and obj.f. in lower panel) during the optimization iteration of the air heater

the flow solver FELCRT, a time accurate solver for fluid flow and heat transfer of incompressible flows. FELCRT is part of the α-FLOW/SX CFD software package 6, specifically developed by NEC for the SX-series of parallel vector computers. The CFD results (r) that are used in the objective function, are the radial, tangential and vertical velocities and the temperatures (m_2=4) in the grid points of the 2.5 m high working space in the room (m_1=828). The desired values (d) of these quantities are 0 m/s, 0 m/s, 0 m/s and 293 K, respectively. The weight factors (w) for each of the result types are all equal to 0.1, such that the objective function is appropriately scaled.

The air flow in the room is simulated until stationary flow is reached. This occurs after about

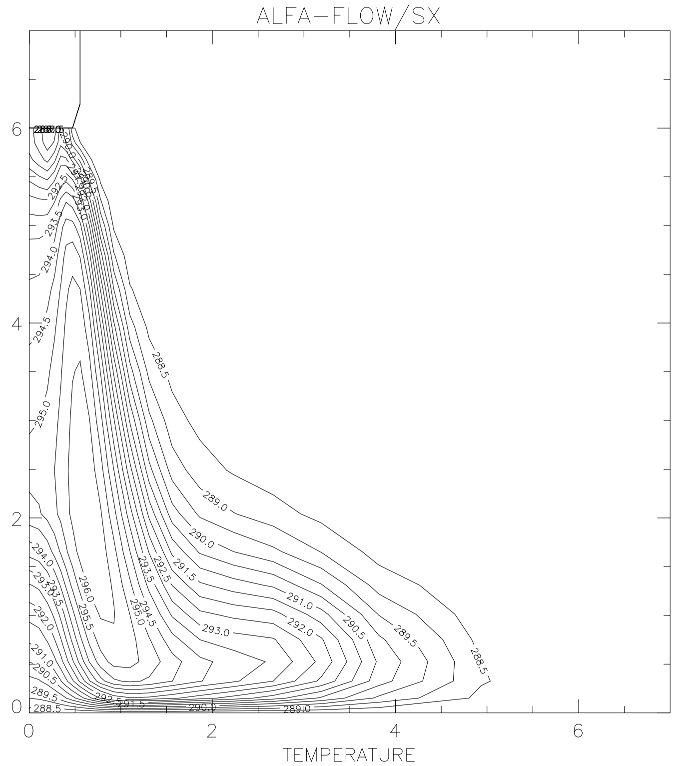


Fig. 4 Temperature distribution in the θ=π/6 plane in the central part of the room (0 m$\leq r \leq$ 7 m ; 0 m$\leq z \leq$ 7 m) for the optimal air heater design

10 s, in approximately 7000 time steps of the flow solver. Residuals have dropped more than 2 orders, which is suffucient for the required engineering accuracy. During the optimization the objective function decreased from an initial value of 204.0 to a minimal value of 78.8, requiring 25 optimization iterations in total, involving 100 CFD simulations. The final values of the design parameters v_r, v_z and T$_{in}$ are 6.6 m/s, -23.2 m/s and 350.0 K, respectively (fig. 3). The temperature distribution in the θ=π/6-plane, calculated for the optimal parameter values is given in fig. 4. In the optimal design the desired temperature and air flow velocities in the working space are approximated, while in the intermediate design stages the hot air of the jets fails to reach the working space due to buoyancy effects.

The total elapsed time of the optimization is 6963 s, in which 25 evaluations of the objective function and sensitivities have been performed, each involving four parallel CFD simulations. The elapsed times of the CFD simulations for the evaluations of the objective function and sensitivities are presented in fig. 5. The average elapsed time of the objective function and sensitivities evaluations is 277 s. Total cumulative computation time for the CFD simulations

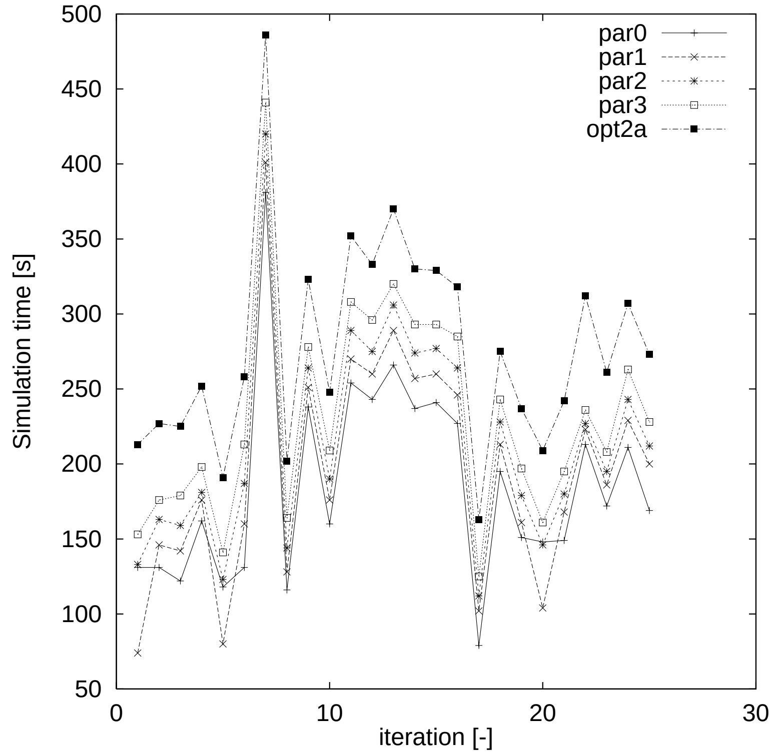


Fig. 5 Computation times of the parallel CFD simulations using the unperturbed (par0) and perturbed (par1, par2 and par3) parameter sets, and total elapsed time of the calculation of objective function and sensitivities (opt2a) for the air heater optimization

is 20721 s, yielding an average CFD computation time of 207 s. Thus, a reduction by a factor 20721/6963=3.0 of the total execution time of the optimization is achieved by the parallelization of the calculations of the objective function and sensitivities.

4 Geometric Airfoil Optimization

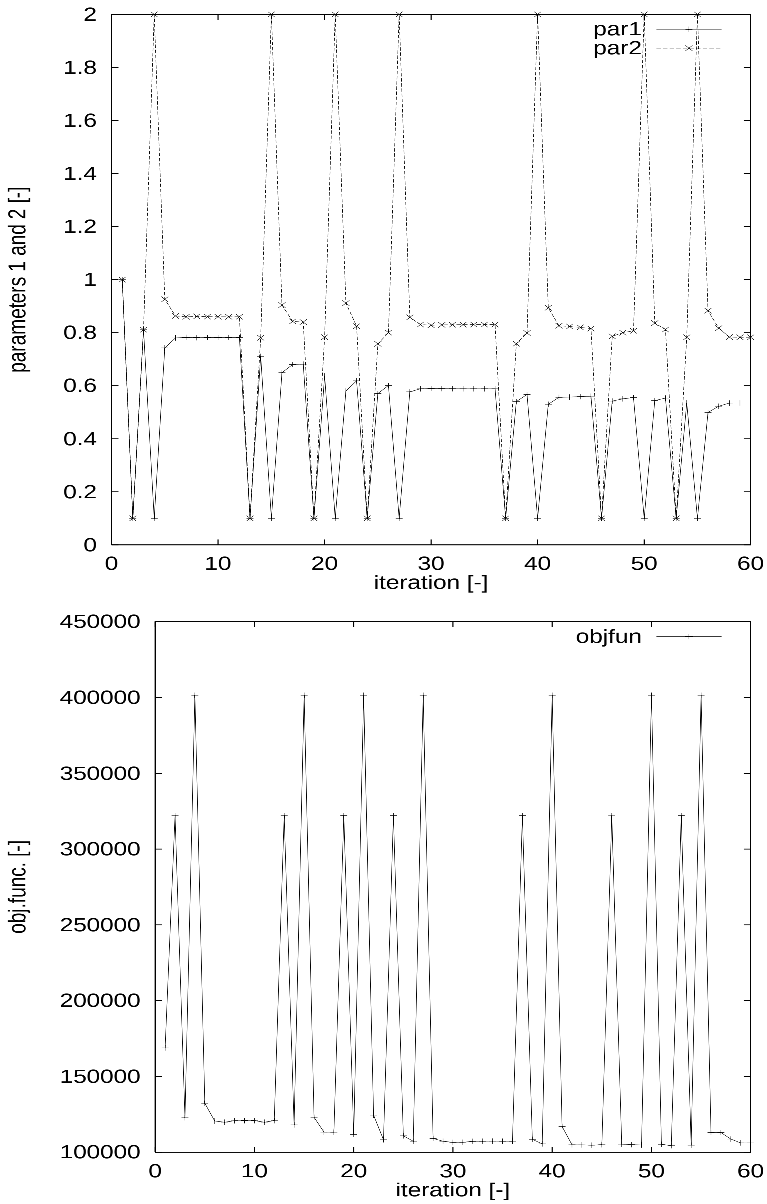


Fig. 6 Design parameters p_1 and p_2 (par1 and par2 in upper panel) and objective function (objfun in lower panel) during the iteration of the airfoil optimization

To illustrate the genericness of the optimization tool a very different application of the tool is presented. Steady compressible turbulent flow around a 2-D airfoil is considered at conditions: free stream Mach number M_∞=0.73, free stream Reynolds number Re_∞=6.5 10^6, and angle of attack α=2.8^o. The objective function consists of the ratio of the lift and drag coefficients: $r_{1,1}$=C_L/C_D ($m_1 = 1$; $m_2 = 1$). The desired value is d_1=100 and weight factor is w_1=10. The

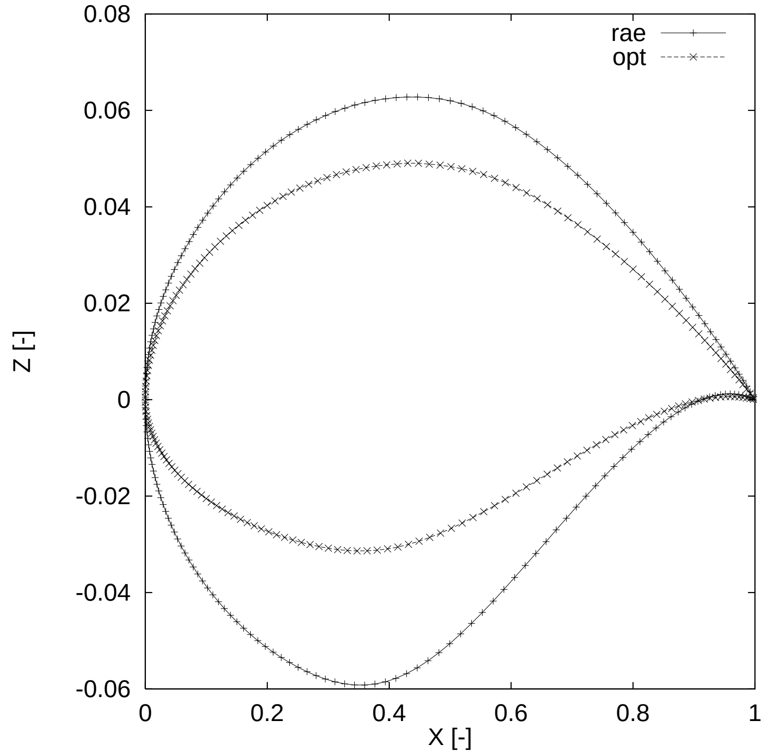
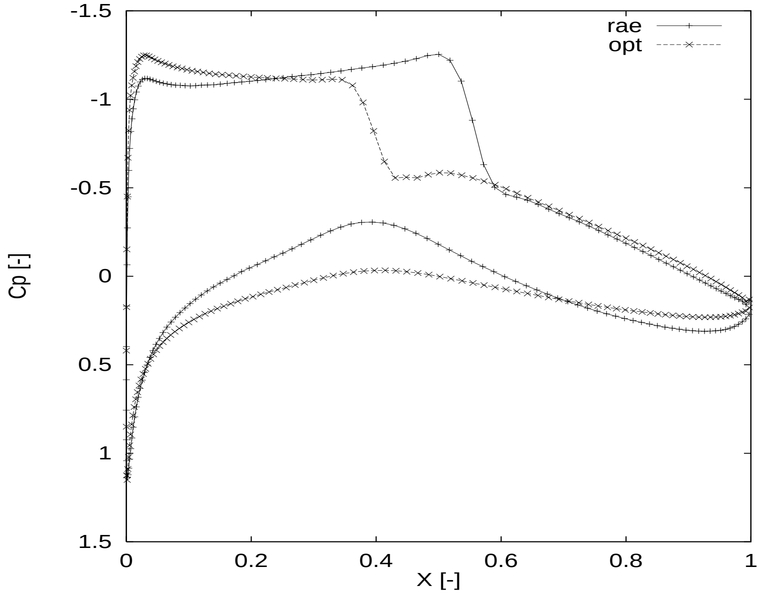


Fig. 7   Original RAE2822 airfoil geometry (rae) and the optimized geometry (opt)

airfoil geometry is based on the RAE2822 airfoil, of which the lower and upper surfaces are defined as a function of the horizontal coordinate x, indicated by $z_l^R(x)$ and $z_u^R(x)$, respectively. In the optimization, the airfoil geometry is transformed by two independent design parameters: one transforming the lower surface ; $z_l(x,p_1) = p_1 \; z_l^R(x)$, and the other transforming the upper surface: $z_u(x,p_2) = p_2 z_u^R(x)$. Initial estimates and lower and upper bounds for the design parameters are 1.0, 0.1, 2.0, respectively, for both p_1 and p_2. In each optimization iteration the transformed airfoil geometry is calculated. A multi-block structured grid with 97 grid points at both the upper and lower surfaces of the airfoil, and containing eight blocks and 9648 cells in total, is generated around this geometry. The new flow solution is calculated, using the solution of the previous optimization iteration as the initial flow field. For each design parameter set these calculations are run sequentially on the SX-4 super computer. In the calculations use is made of the ENFLOW flow simulation system 7 which has been developed at NLR: the grid generator ENGRID and the Euler/Navier-Stokes equations flow solver ENSOLV for 3-D multi-block structured grids. The thin-layer Reynolds-averaged Navier-Stokes equations, closed by the Cebeci-Smith turbulence model, are solved by an explicit time-marching finite-volume technique with adaptive numerical dissipation in combination with a three-level multigrid algorithm. The flow solutions are calculated iteratively until C_L has converged to an order 10^{-4}.



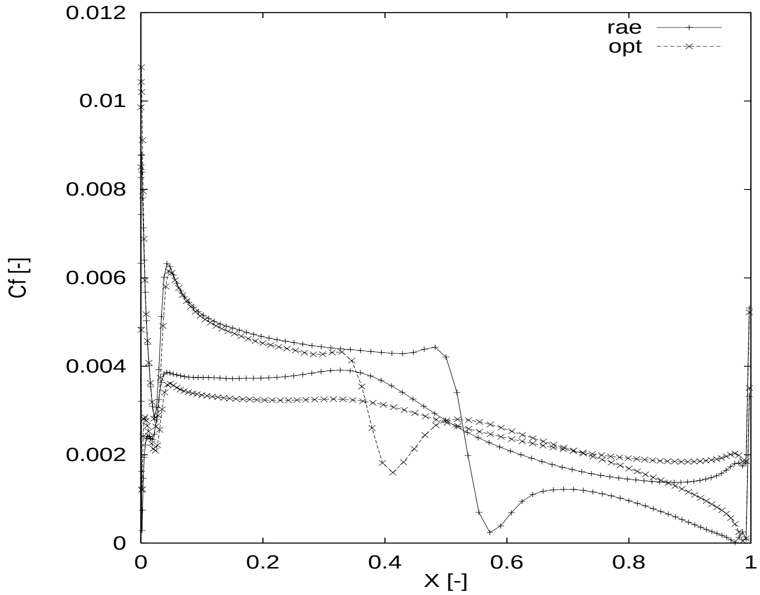


Fig. 8 Pressure coefficient (upper panel) and skin friction coefficient (lower panel) of original RAE2822 airfoil (rae) and optimized airfoil (opt)

C_L and C_D are calculated from the air flow around the airfoil. The initial estimates of the parameter values, 1.0 and 1.0, respectively, represent the original RAE2822 airfoil. For this airfoil C_L=0.7797 and C_D=0.0189 were calculated, yielding a C_L/C_D-ratio of about 41.2. The parameters were adapted in 60 optimization iterations to the optimal values of 0.535 and 0.783, respectively. For the optimal airfoil it was found that C_L=0.7859 and C_D=0.0145, yielding a C_L/C_D-ratio of about 54.2 (fig. 6). The optimal airfoil is significantly flatter than the original

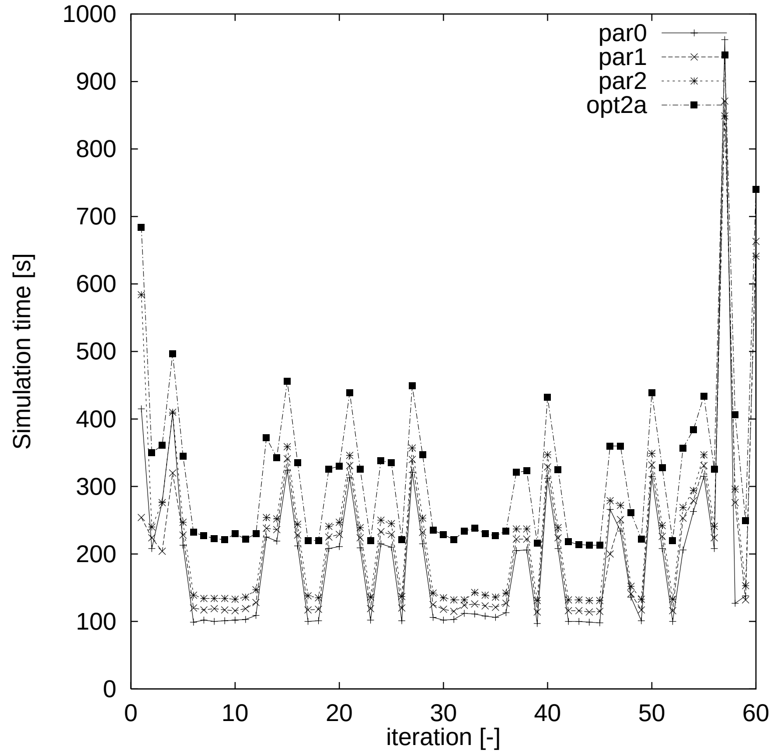


Fig. 9 Computation times of the parallel CFD simulations of the unperturbed (par0) and perturbed (par1 and par2) parameter sets, and total elapsed time of the calculation of objective function and sensitivities (opt2a) for the airfoil optimization

RAE2822 airfoil (fig. 7). Not only the slight increase of C_L of about 0.8 %, but mainly the strong decrease of C_D of about 23 %, are responsible for the decrease of the C_L/C_D-ratio, and as such for the improved design. The decrease of C_D is largely due to the weaker shock (fig. 8); the skin-friction drag coefficient slightly increases about 1.8 % from 0.0055 to 0.0056 (fig. 8).

60 optimization iterations were required, in which 180 CFD simulations have been performed, in a total elapsed time of 19447 s (fig. 9). Total cumulative computation time for the CFD simulations is 38717 s, yielding an average CFD computation time of 215 s. The reduction factor achieved by the parallelization of the calculations of the objective function and sensitivities is 38717/19447=2.

5 Discussion

The optimization tool has been used successfully in design optimization involving CFD analysis. Two different design problems in which totally different flow solvers have been used, have been presented to illustrate the possibilities of the tool, stressing its genericness and computational performance.

In both optimizations major and minor iterations have been performed. In the minor iterations a small step in the local search direction is taken, i.e., a small update of the parameter values (figs. 3, 6). In the major iterations a large step is taken in order to escape from the convergence to local sub-minima of the objective function by the minor iterations. The large variations of the parameter values in the major iterations cause an increase of the CFD computation times in the airfoil optimization, due to the use of the solution of the previous iteration as the initial flow field and the convergence criterion (fig. 9). The large CFD computation times in the seventh iteration of the air heater optimization is due to the parameter value v_z=-30 m/s, which causes very small time steps, and thus slow convergence, in the time integration of the CFD solver. (fig. 5).

It should be noted that the elapsed times of the CFD computations presented in figs. 5 and 9 also include some pre- and post-processing of the CFD simulations, which is perfomed sequentially. As such the almost constant differences in computation times of of the CFD jobs for each of the parameter sets (par0, par1, par2 and par3 in figs. 5 and 9) can be explained by the cumulating elapsed time of the pre- and post-processing of the CFD jobs. Moreover, in the airfoil optimization the geometry transformation and grid generation, which are also performed sequentially, are included in the total elapsed time (opt2a in fig. 9), which explains the rather large overhead time in this optimization (difference between the opt2a curve and the par0/1/2 curves in fig. 9).

The large peaks in the computation times in the 57th and 60th iterations of the airfoil optimization (fig. 5) are due to the occupation of all the processors of the SX-4 by other processes, causing the submitted CFD jobs to wait in the queue.

Acknowledgements

We thank Drs. P. Wijnandts and Dr.ir. J.C. Kok for their support in the geometric airfoil optimization study.

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